

Sarcosine, N-pentafluoropropionyl-, hexadecyl ester

Inchi:	InChI=1S/C22H38F5NO3/c1-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-31-19(29)18-28(2)20
InchiKey:	GSGCQKPYPJZCRY-UHFFFAOYSA-N
Formula:	C22H38F5NO3
SMILES:	CCCCCCCCCCCCCCCCOC(=O)CN(C)C(=O)C(F)(F)C(F)(F)F
Mol. weight [g/mol]:	459.54

Physical Properties

Property code	Value	Unit	Source
hfus	60.71	kJ/mol	Joback Method
hvap	108.25	kJ/mol	Cheméo Relay (1.0)
log10ws	-6.94		Cheméo Relay (1.0)
logp	6.667		Crippen Method
mcvol	348.680	ml/mol	McGowan Method
rinpol	2422.00		NIST Webbook
tb	604.66	K	Cheméo Relay (1.0)
tf	295.16	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1141.34	J/mol×K	835.25	Joback Method
cpg	1159.86	J/mol×K	866.62	Joback Method
cpg	1177.27	J/mol×K	897.99	Joback Method
cpg	1193.66	J/mol×K	929.36	Joback Method
cpg	1209.10	J/mol×K	960.73	Joback Method
cpg	1223.65	J/mol×K	992.10	Joback Method
cpg	1237.40	J/mol×K	1023.47	Joback Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U320944&Units=SI>

Joback Method: https://en.wikipedia.org/wiki/Joback_method

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Legend

cpg:	Ideal gas heat capacity
hfus:	Enthalpy of fusion at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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